The CA Lexicon is now available in the Controlled Term (/CT) field.
Enter HELP LEXICON for full details.


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=> s l15
L17          0 L15

=> dis his

     (FILE 'HOME' ENTERED AT 22:52:28 ON 12 AUG 2001)

     FILE 'REGISTRY' ENTERED AT 22:52:35 ON 12 AUG 2001
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FUL
L4             STRUCTURE UPLOADED
L5          27 S L4 FUL

     FILE 'CAPLUS' ENTERED AT 22:55:33 ON 12 AUG 2001
L6          21 S L5

     FILE 'REGISTRY' ENTERED AT 23:00:12 ON 12 AUG 2001
L7             STRUCTURE UPLOADED
L8           0 S L7 FUL
L9             STRUCTURE UPLOADED
L10          0 S L9 FUL
L11            STRUCTURE UPLOADED
L12            STRUCTURE UPLOADED
L13          0 S L12 FUL

     FILE 'CAPLUS' ENTERED AT 23:09:00 ON 12 AUG 2001

     FILE 'REGISTRY' ENTERED AT 23:17:13 ON 12 AUG 2001
L14            STRUCTURE UPLOADED
L15          0 S L14
L16          9 S L14 FUL

     FILE 'CAPLUS' ENTERED AT 23:23:36 ON 12 AUG 2001
L17          0 S L15

=> s l16
L18         14 L16

=> d 1-5 bib abs

L18  ANSWER 1 OF 14  CAPLUS  COPYRIGHT 2001 ACS
AN   2001:152645  CAPLUS
DN   134:193224
TI   Fluorenone compounds with modified 7-position substituents for treating
     and preventing brain and spinal injury
IN   Cragoe, Edward J., Jr.; Marangos, Paul J.; Weimann, Torsten R.
PA   Questcor Pharmaceuticals, Inc., USA
SO   PCT Int. Appl., 66 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
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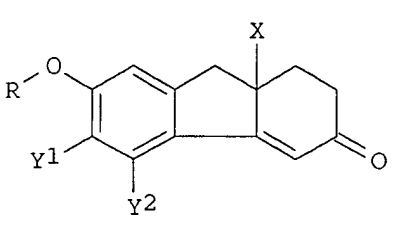
PI WO 2001014334 A1 20010301 WO 2000-US22990 20000822
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
US 6251898 B1 20010626 US 1999-379656 19990824
PRAI US 1999-379656 A 19990824
US 1999-379816 A 19990824
OS MARPAT 134:193224
GI



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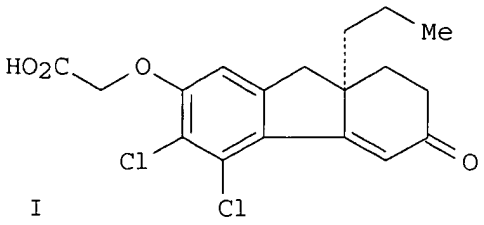

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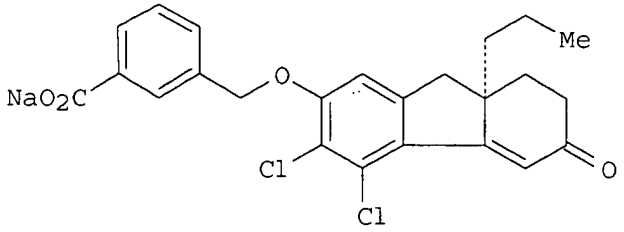


III

AB New neuroprotective drugs are disclosed, which are analogs of certain previously known fluorenone compds. The new analogs have structure I [where X is a lower alkyl, substituted alkyl, or cycloalkyl group, R is selected from certain types of ether, ester, or amide groups, and Y1 and Y2 are halogen, H, or Me]. I potently inhibit the unwanted release of excitotoxins by astrocyte cells following an injury or insult to the brain or spinal cord. The compds. are more than 30 times more potent than the previously known lead compd., L-644,711 (II), in reducing aspartate release by stressed astrocyte cells. I can also help reduce swelling in astrocyte cells, and can thereby help promote proper blood flow through the brain following a head injury or other crisis. Accordingly, I can reduce brain or spinal cord damage caused by a hypoxic, ischemic, infective, inflammatory, or other injury, crisis, or insult to the brain or spinal cord. As an illustration, several examples were prepd. and tested. For instance, cleavage of the carboxymethyl group from II (ref. given) gives a phenolic intermediate, which was re-etherified with Me 3-(bromomethyl)benzoate and then sapond. to give the sodium salt III. I were very efficacious in several in vitro animal models of focal or global brain ischemia. In a test for suppression of excitotoxin release by stressed astrocytes, III had a potency of 3,378% compared to the benchmark compd. II (100%). The structure-activity relationship resulting in the increased potency of the new compds. is described.

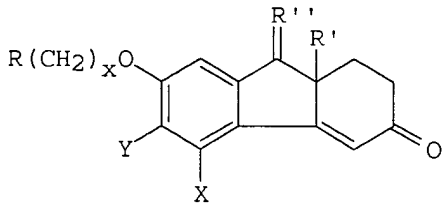
RE.CNT 4
RE

(1) Cragoe; US 4356313 A 1982 CAPLUS
(2) Cragoe; US 4731471 A 1998 CAPLUS
(3) Pietruszkiewicz; US 4731470 A 1988 CAPLUS
(4) Woltersdorf; US 4797391 A 1989 CAPLUS

L18 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2001 ACS
AN 1989:496878 CAPLUS
DN 111:96878
TI Preparation of [(5,6-dichloro-3-oxo-9,9a-disubstituted-2,3,9,9a-tetrahydrofluoren-7-yl)oxy]alkanoic acids and -alkanimidamides and their pharmaceutical compositions for treatment of gray matter edema
IN Woltersdorf, Otto W., Jr.; Cragoe, Edward J., Jr.; Pietruszkiewicz, Adolph M.
PA Merck and Co., Inc., USA
SO U.S., 15 pp. Cont. of U. S. Ser. No. 910,924, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4797391	A	19890110	US 1988-150462	19880208

PRAI US 1986-910924 19860924
OS MARPAT 111:96878
GI



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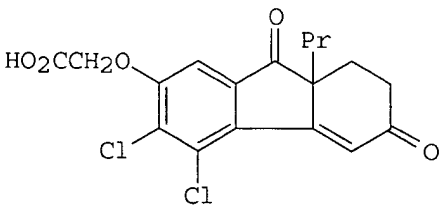


II

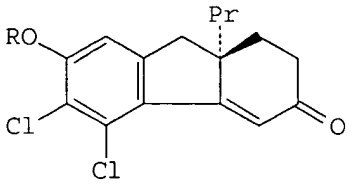
AB The title compds. [I; R = CO2R1, C(:R3)R2; R' = alkyl, (halo)aryl, aralkyl, cycloalkyl, cycloalkylalkyl; R'' = O, or H plus OH, Cl, Br, Me, NH2, N3, alkanoyloxy, or NHP(O)(OEt)2; R1 = H, alkyl, carboxyalkyl; R2 = NH2, NHR4, NR4R5; R3 = NH, NR4; R4, R5 = alkyl, amino (R4 and R5 may not both be amino); R2R3, R4R5 may form rings; X, Y = halo, alkyl; x = 1-4] and related compds. were prepd. as agents for treating brain edema (no data). 5,6-Dichloro-1,2,9,9a-tetrahydro-7-methoxy-9a-propyl-3H-fluoren-3-one underwent successive benzylic bromination with NBS, hydrolysis of the 9-bromo deriv. by AgNO2 in aq. MeOCH2CH2OH, Jones oxidn. of the 9-alc., demethylation of 7-MeO by pyrolysis with pyridine-HCl, alkylation of 7-OH by BrCH2CO2Et and K2CO3 in DMF, and sapon. by aq. NaOH/EtOH, to give (fluorenyloxy)acetic acid II. A parenteral soln. of II.Na was prepd. from 500 mg II, 5.6 mL 0.25 N NaHCO3, and H2O to make 10 mL.

L18 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2001 ACS
AN 1988:167131 CAPLUS

DN 108:167131
TI Preparation of an enantiomer of a substituted fluorenyloxyacetic acid for treating brain edema
IN Conn, Robin S. E.; Karady, Sandor
PA Merck and Co., Inc., USA
SO U.S., 6 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4704472	A	19871103	US 1985-797311	19851218

PI
GI



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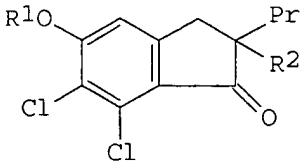


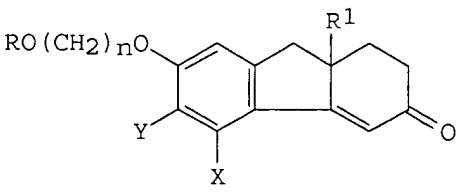
III

AB The title acid (I; R = CH2CO2H) (II), useful in treating brain edema (no data), is prepd. Stirring a mixt. of indanone III (R1 = Me, R2 = H) with MeCOCH:CH2, dihydro-3,4-dichlorobenzylcinchonidinium chloride, and KOH in MePh gave 92% III (R1 = Me, R2 = MeCOCH2CH2) as a 70 : 30 R- and S-isomer mixt. which was cyclized with H2SO4 at 65-75.degree. to give the phenolic I (R = H) (IV) after hydrolysis over SlCl3 in situ. Substitution of IV with ClCH2CO2Et over K2CO3, NaI, and Triton X-405 gave 96.6% ester I (R = CH2CO2Et) which was sapond. to give 89.8% II as a 76:24 R- and S-isomer mixt.

L18 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2001 ACS
AN 1987:515380 CAPLUS
DN 107:115380
TI Preparation of [(5,6-dichloro-3-oxo-9a-propyl-2,3,9,9a-tetrahydrofluoren-7-yl)oxy]ethanol and its derivatives as agents for treating brain injuries
IN Cragoe, Edward J., Jr.
PA Merck and Co., Inc. , USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4675341	A	19870623	US 1986-896022	19860813

PI
GI



I

AB Title compds. I [X, Y = halo, alkyl; R = H, C(O)(CH2)mNMe2,

C(O)CH2CH2CO2H, C(O)CH:CH2CO2H; R1 = alkyl, cycloalkyl, aralkyl, (halo)aryl; n = 1-4; m = 1-3] are prepd. as agents used for treating brain injury (no data). A mixt. contg. 3.36 mmol each of DBN and 4-(dimethylamino)butyric acid hydrochloride and also (R)-(+)-[(5,6-dichloro-1,2,9,9a-tetrahydro-9a-propyl-1H-fluoren-7-yl)oxy]ethanol (amt. not specified) was stirred for 16 h to give 1.03 g I [X = Y = Cl, R = Me2N(CH2)3C(O), R1 = Pr, n = 2] (II). Capsules were formulated contg. II 108.4, lactose 90.6, and Mg stearate 1 mg/capsule.

L18 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2001 ACS
AN 1987:156087 CAPLUS
DN 106:156087
TI [(2,3,9,9a-Tetrahydro-3-oxo-9a-substituted-1H-fluoren-7-yl)oxy]ethanimidamides and [(2,3,9,9a-tetrahydro-3-oxo-9a-substituted-1H-fluoren-7-yl)oxy]ethanimidic acid hydrazides, their derivatives and their salts
IN Cragoe, Edward J., Jr.; Woltersdorf, Otto W., Jr.
PA Merck and Co., Inc. , USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4604396	A	19860805	US 1985-780145	19850926
	CA 1284329	A1	19910521	CA 1986-518544	19860918
	DK 8604572	A	19870327	DK 1986-4572	19860925
	EP 217287	A2	19870408	EP 1986-113183	19860925
	EP 217287	A3	19880720		
	EP 217287	B1	19910626		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	ES 2001801	A6	19880616	ES 1986-2184	19860925
	AT 64733	E	19910715	AT 1986-113183	19860925
	JP 62084052	A2	19870417	JP 1986-226326	19860926
PRAI	US 1985-780145		19850926		
	EP 1986-113183		19860925		

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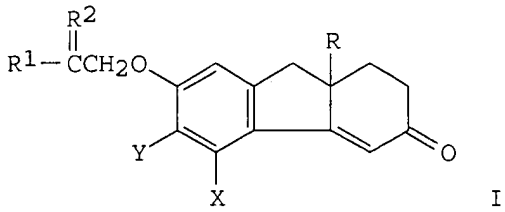
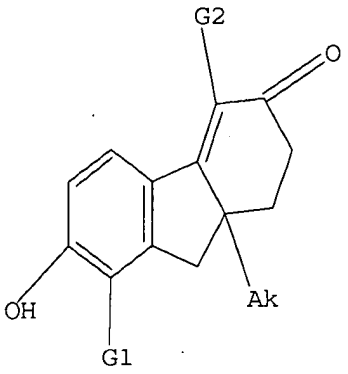


I

AB Title compds. I (R = alkyl, aryl, haloaryl, aralkyl, cycloalkyl, cycloalkylalkyl; R1 = NH2, NHR3, NR3R4; R2 = NH, NR3; R3, R4 = alkyl, amino; wherein R1 and R2 may be joined together via R3 to form a heterocyclic ring of 5 or 6 atoms contg. 2N; NR3R4 = heterocycle; X, Y = halo, alkyl); and their pharmaceutically acceptable salts, useful in the treatment of gray matter edema, are prepd. I are devoid of the pharmacodynamic, toxic, or various side effects characteristic of the diuretics, steroids, and barbiturates used in current therapy. Thus, [R-(+)]-5,6-dichloro-9a-propyl-7-hydroxy-2,3,9,9a-tetrahydro-1H-fluoren-3-one was treated with K2CO3 and ClCH2CN to give the fluorenyloxyacetonitrile deriv., which was treated first with NaOMe and then with NH4Cl to give [R-(+)]-I.HCl(R = Pr, R1 = NH2, R2 = NH, X = Y =

=> d
L14 HAS NO ANSWERS
L14 STR



G1 H,CF2,OH,Cl,F
G2 H,Me,Et,n-Pr,CF3,CN,C(O)CH3,Cl

Structure attributes must be viewed using STN Express query preparation.

=> s l14
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SAMPLE SCREEN SEARCH COMPLETED - 24100 TO ITERATE

4.1% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 472755 TO 491245
PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14

=> s l14 ful
FULL SEARCH INITIATED 23:22:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 488090 TO ITERATE

82.0% PROCESSED 400000 ITERATIONS 9 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.16

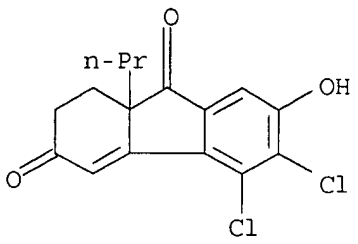
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 488090 TO 488090
PROJECTED ANSWERS: 9 TO 19

L16 9 SEA SSS FUL L14

=> d 1-9

L16 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 121913-84-6 REGISTRY
CN 1H-Fluorene-3,9(2H,9aH)-dione, 5,6-dichloro-7-hydroxy-9a-propyl- (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C16 H14 Cl2 O3
SR CA

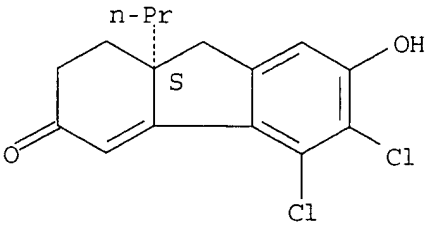
LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L16 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 105615-51-8 REGISTRY
CN 3H-Fluoren-3-one, 5,6-dichloro-1,2,9,9a-tetrahydro-7-hydroxy-9a-propyl-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H16 Cl2 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)

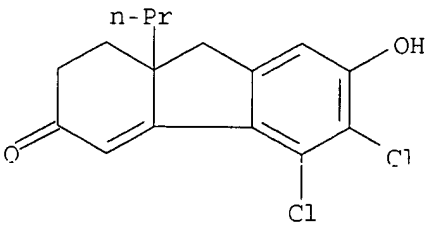
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L16 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 101833-21-0 REGISTRY
CN 3H-Fluoren-3-one, 5,6-dichloro-1,2,9,9a-tetrahydro-7-hydroxy-9a-propyl-, (+)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H16 Cl2 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

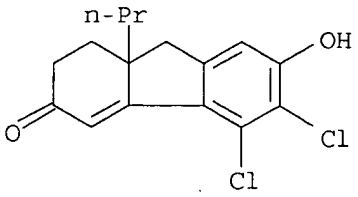
Rotation (+).



1 REFERENCES IN FILE CA (1967 TO DATE)

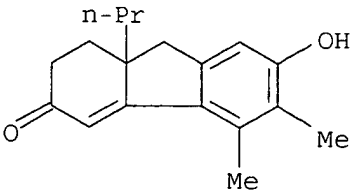
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L16 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 101469-43-6 REGISTRY
CN 3H-Fluoren-3-one, 5,6-dichloro-1,2,9,9a-tetrahydro-7-hydroxy-9a-propyl-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3H-Fluoren-3-one, 5,6-dichloro-1,2,9,9a-tetrahydro-7-hydroxy-9a-propyl-, (.+-.)-
FS 3D CONCORD
MF C16 H16 Cl2 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

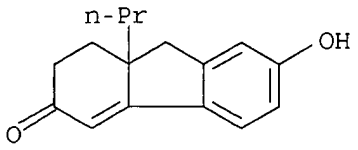
L16 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 101375-45-5 REGISTRY
CN 3H-Fluoren-3-one, 1,2,9,9a-tetrahydro-7-hydroxy-5,6-dimethyl-9a-propyl-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3H-Fluoren-3-one, 1,2,9,9a-tetrahydro-7-hydroxy-5,6-dimethyl-9a-propyl-, (.+-.)-
FS 3D CONCORD
MF C18 H22 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L16 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 101375-44-4 REGISTRY
CN 3H-Fluoren-3-one, 1,2,9,9a-tetrahydro-7-hydroxy-9a-propyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3H-Fluoren-3-one, 1,2,9,9a-tetrahydro-7-hydroxy-9a-propyl-, (.+-.)-
FS 3D CONCORD
MF C16 H18 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L16 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 101165-87-1 REGISTRY
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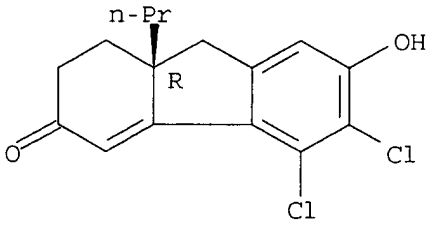
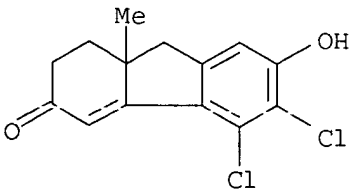
OTHER CA INDEX NAMES:
CN 3H-Fluoren-3-one, 5,6-dichloro-1,2,9,9a-tetrahydro-7-hydroxy-9a-propyl-, (R)-
FS STEREOSEARCH
MF C16 H16 Cl2 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



6 REFERENCES IN FILE CA (1967 TO DATE)
6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L16 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 84226-62-0 REGISTRY
CN 3H-Fluoren-3-one, 5,6-dichloro-1,2,9,9a-tetrahydro-7-hydroxy-9a-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3H-Fluoren-3-one, 5,6-dichloro-1,2,9,9a-tetrahydro-7-hydroxy-9a-methyl-, (.+-.)-
FS 3D CONCORD
MF C14 H12 Cl2 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)



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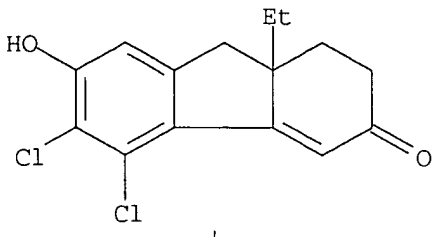
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L16 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2001 ACS
RN 81997-15-1 REGISTRY
CN 3H-Fluoren-3-one, 5,6-dichloro-9a-ethyl-1,2,9,9a-tetrahydro-7-hydroxy-
(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3H-Fluoren-3-one, 5,6-dichloro-9a-ethyl-1,2,9,9a-tetrahydro-7-hydroxy-,
(.+-.)-
DR 79796-62-6
MF C15 H14 Cl2 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)



7 REFERENCES IN FILE CA (1967 TO DATE)
7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	150.16	898.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-15.29

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FILE COVERS 1947 - 12 Aug 2001 VOL 135 ISS 8
FILE LAST UPDATED: 10 Aug 2001 (20010810/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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